

FIG. 1(a)

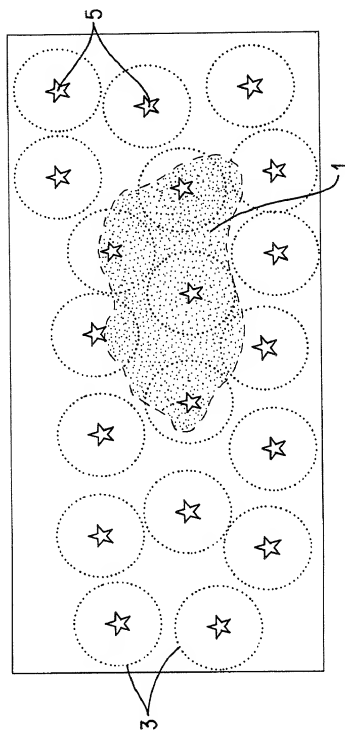


FIG. 1(b)

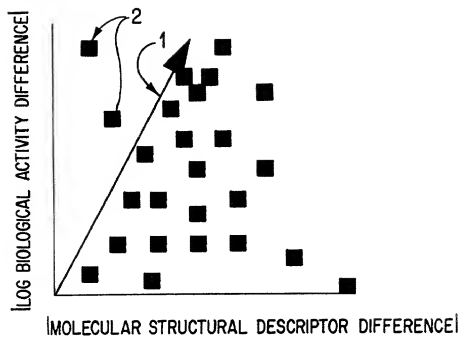


FIG. 2

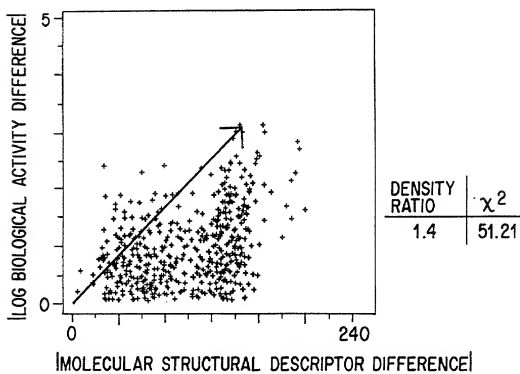
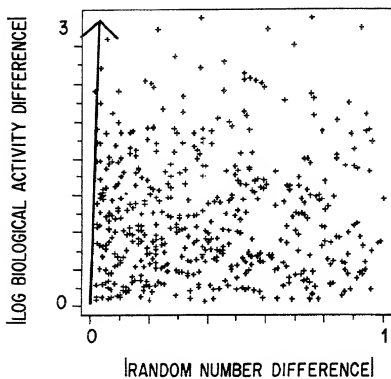
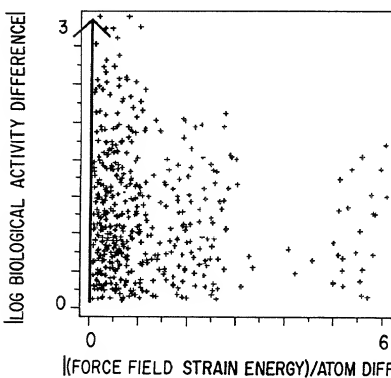


FIG. 3



DENSITY RATIO	χ^2
1.00	0.00

FIG. 4



DENSITY RATIO	χ^2
0.96	0.46

FIG. 5

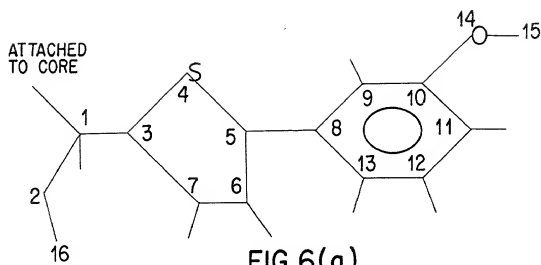


FIG. 6(a)

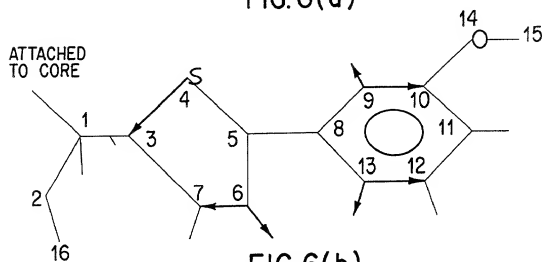


FIG. 6(b)

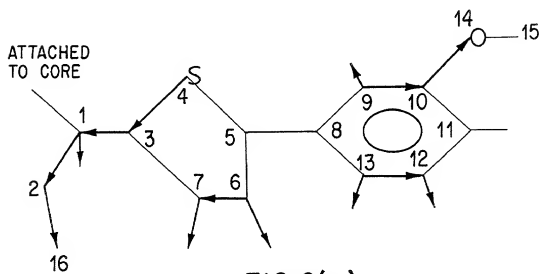


FIG. 6(c)

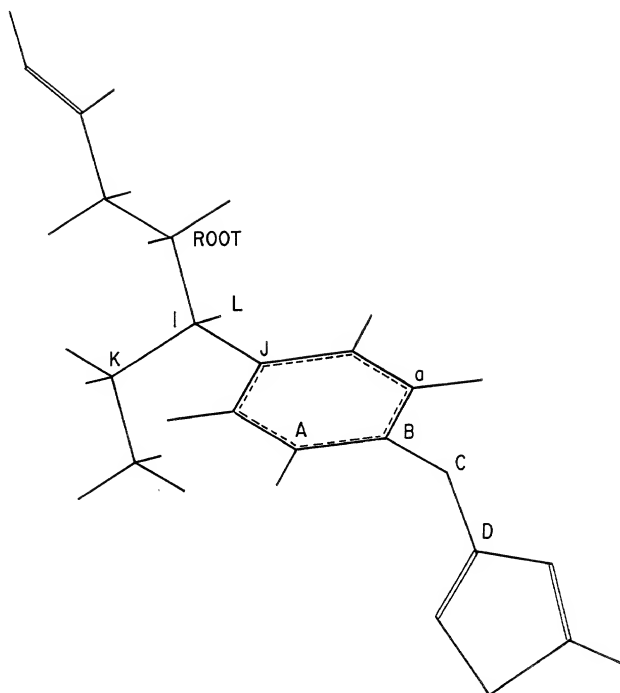


FIG. 6(d)

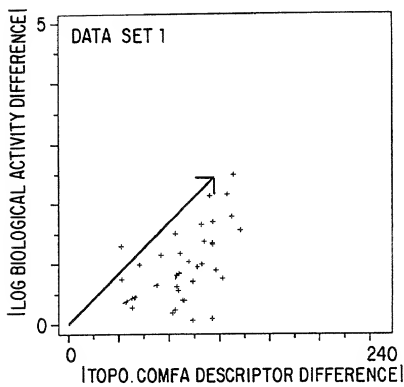


FIG.7(a)

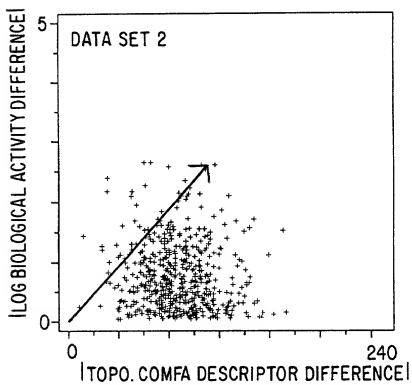


FIG.7(b)

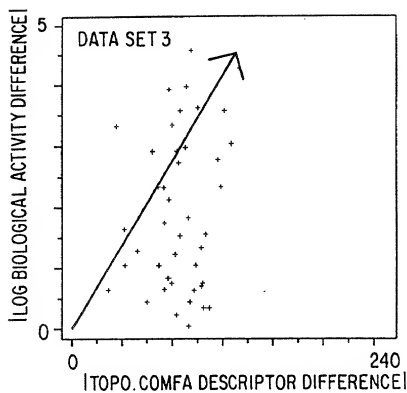


FIG.7(c)

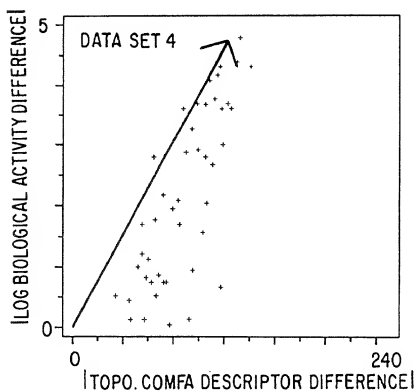


FIG.7(d)

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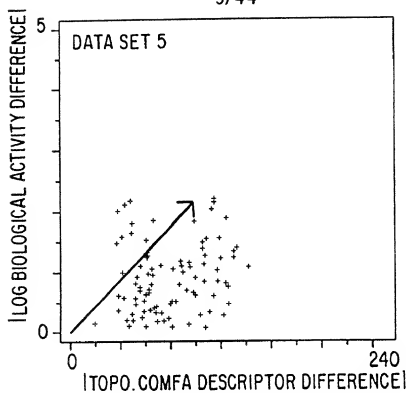


FIG.7(e)

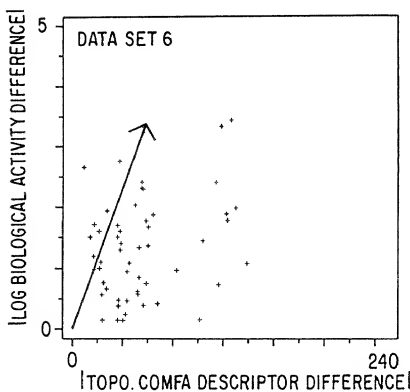


FIG.7(f)

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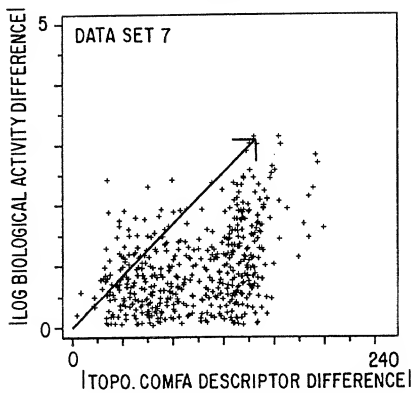


FIG.7(g)

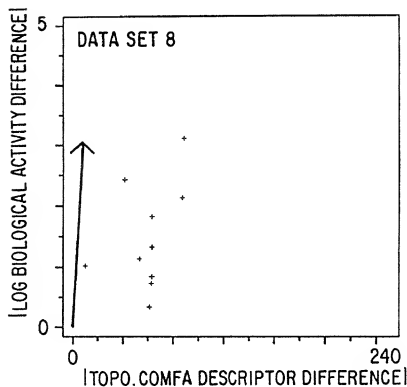


FIG.7(h)

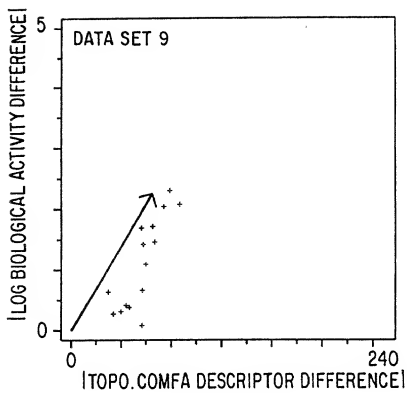


FIG. 7(i)

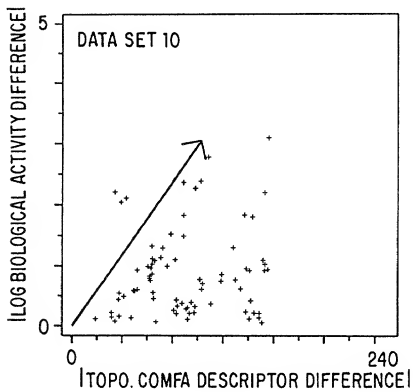


FIG. 7(j)

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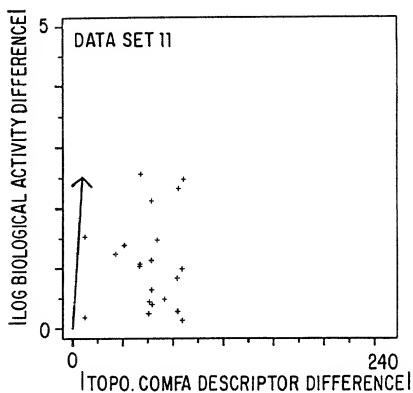


FIG.7(k)

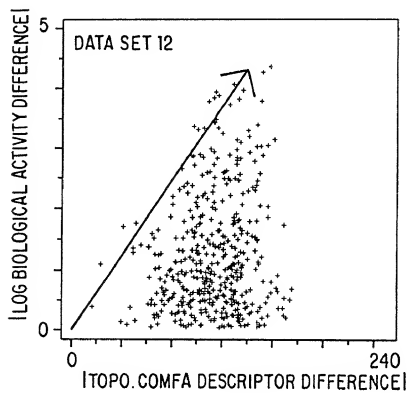


FIG.7(l)

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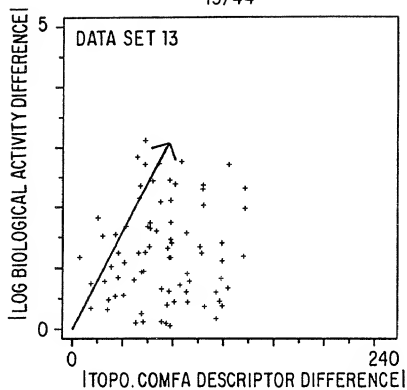


FIG.7(m)

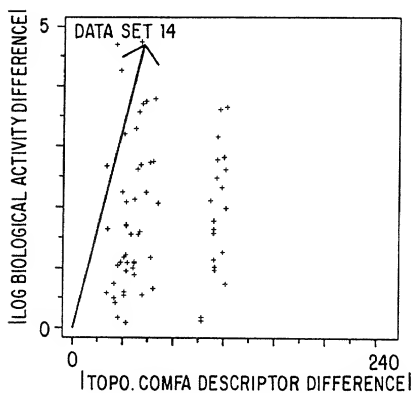


FIG.7(n)

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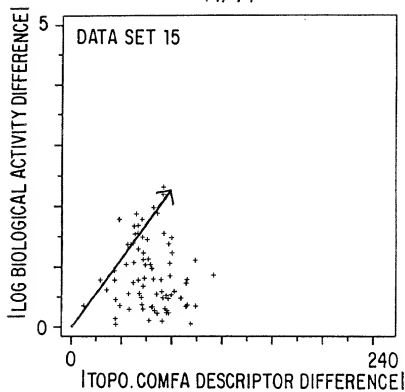


FIG.7(o)

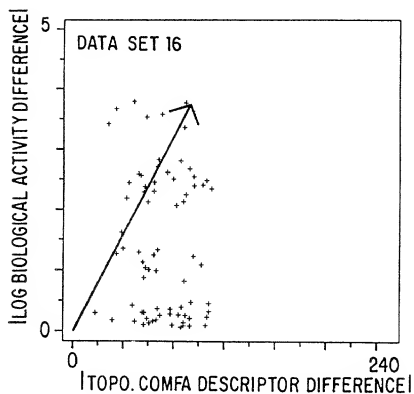


FIG.7(p)

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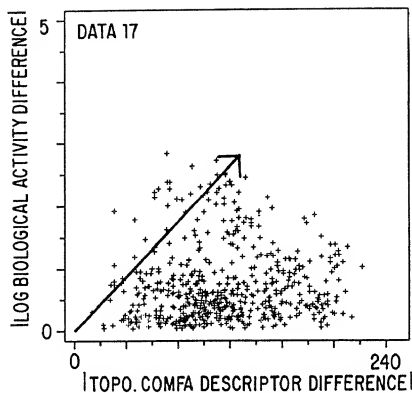


FIG.7(q)

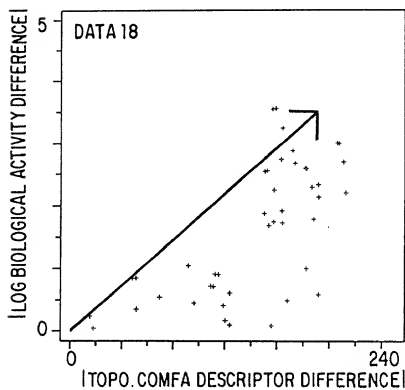


FIG.7(r)

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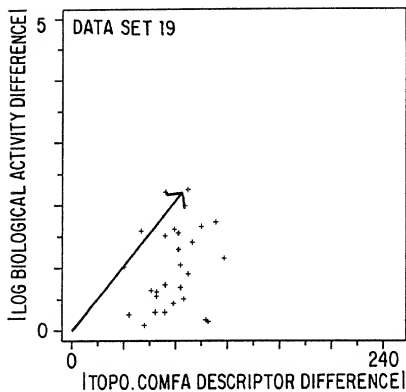


FIG. 7(s)

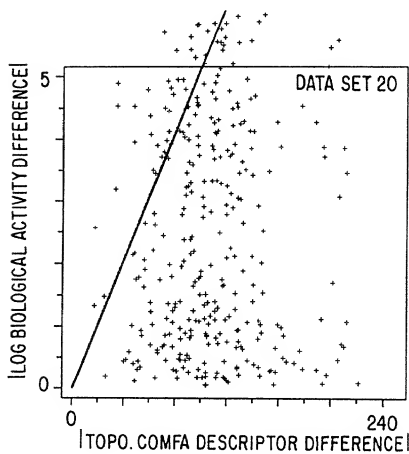
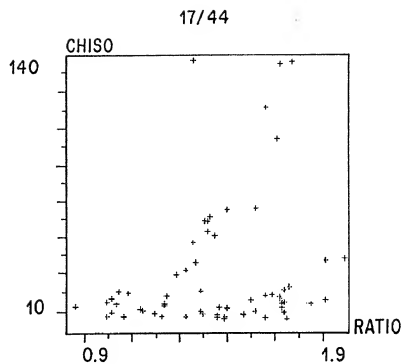
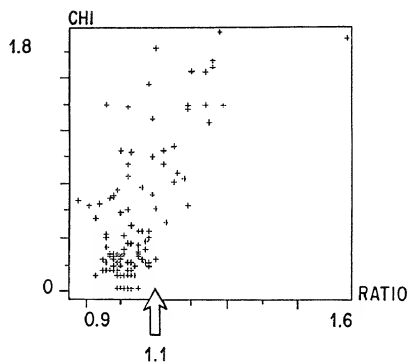


FIG. 7(t)



1.1

FIG. 8(a)



1.1

FIG. 8(b)

0066145-05201

105250-961990

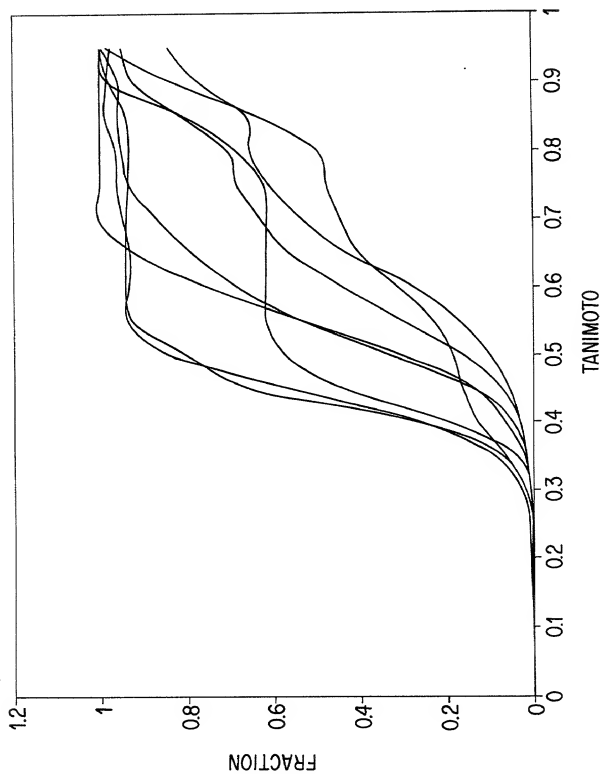


FIG. 9(a)

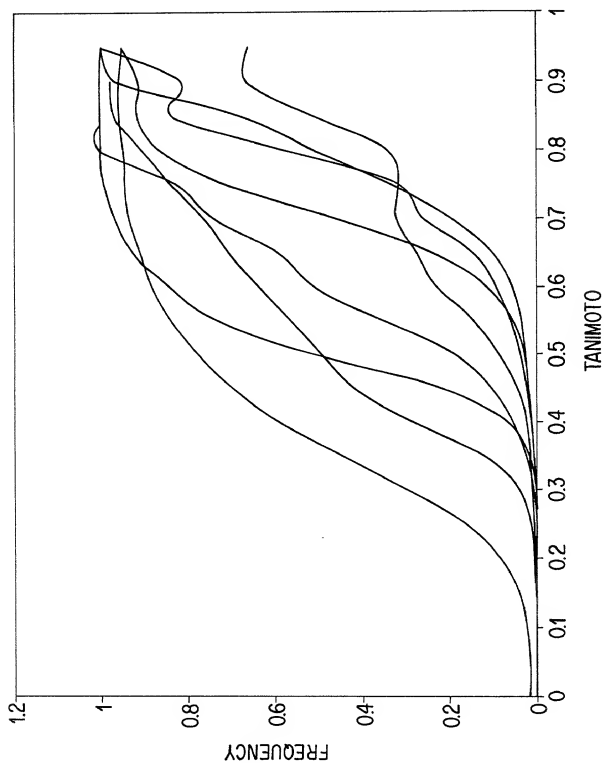


FIG. 9(b)

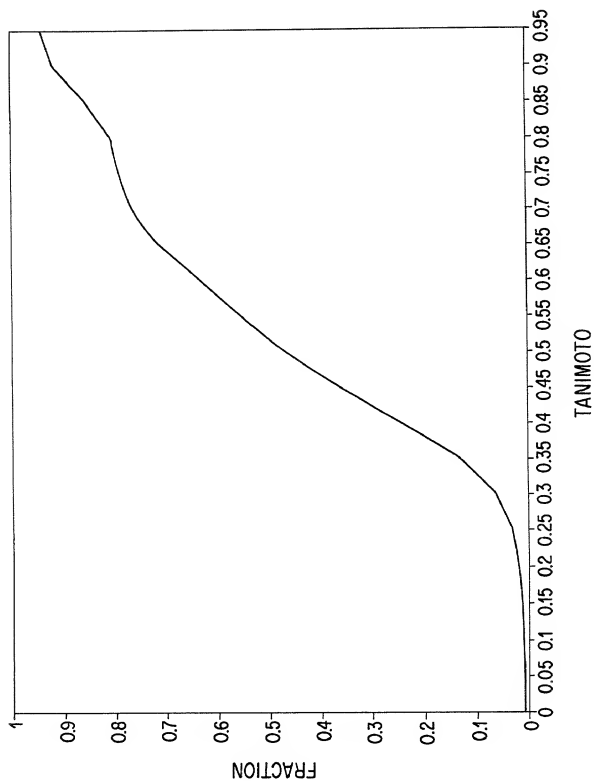


FIG. 9(c)

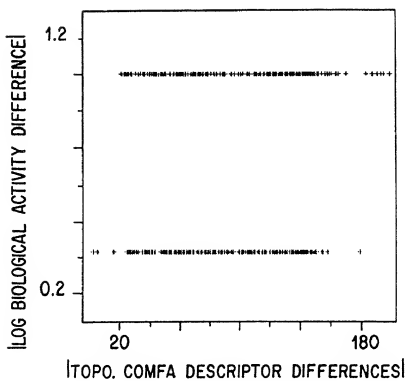


FIG.10(a)

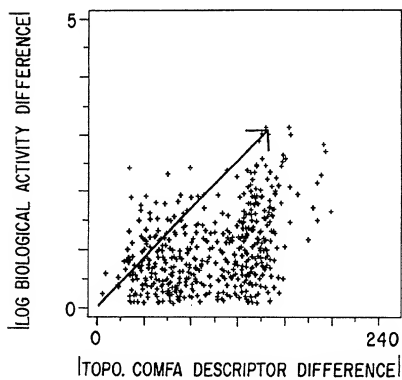


FIG.10(b)

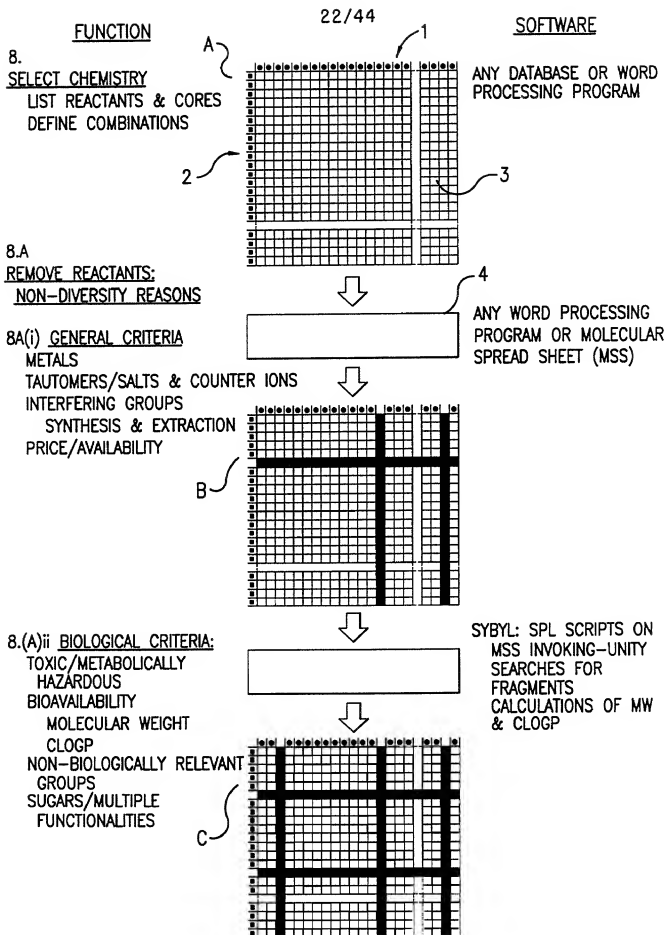


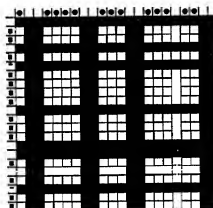
FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION
 TOPOMERIC CONFORMER
 ALIGNMENT
 CoMFA FIELD GENERATION:
 HYDROGEN BOND FIELD
 GENERATION
 ROTATABLE BOND FIELD
 ATTENUATION
 CALCULATE FIELD
 DIFFERENCES
 CLUSTER
 REACTANT SELECTION FROM
 EACH CLUSTER

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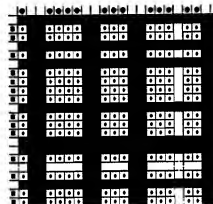
SYBYL: SELECTOR &
 CONCORD 3.2.1
 SPECIALIZED SOFTWARE:
 APPENDIX "A"
 (SYBYL: CoMFA
 STERIC & MSS)

SYBYL: HIERCHICAL
 CLUSTER - MSS
 SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS

E

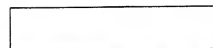


SYBYL: LEGION MSS

8D

REMOVE PRODUCTS:NON-DIVERSITY REASONS

GENERAL CRITERIA:



F

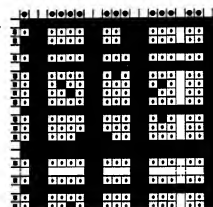
SYBYL: SPL SCRIPTS
 ON MSS

FIG.11(b)

00866405 102500 5049880

8D

BIOLOGICAL CRITERIA:

METABOLICALLY HAZARDOUS

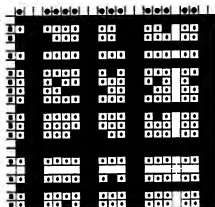
BIOAVAILABILITY

MOLECULAR WEIGHT

CLOGP

SYBYL: SPL SCRIPTS ON
MSS INVOKING -
UNITY SEARCHES FOR
FRAGMENTS
CALCULATIONS OF MW
& CLOGP

G



8E

REMOVE NON-DIVERSE
PRODUCTS:

GENERATE Tanimoto
2D FINGERPRINTS

SAMPLE PRODUCTS:

EXCLUDE TAN ≥ 0.85

UNITY

H

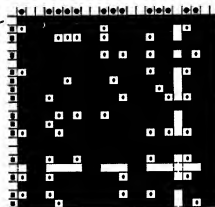
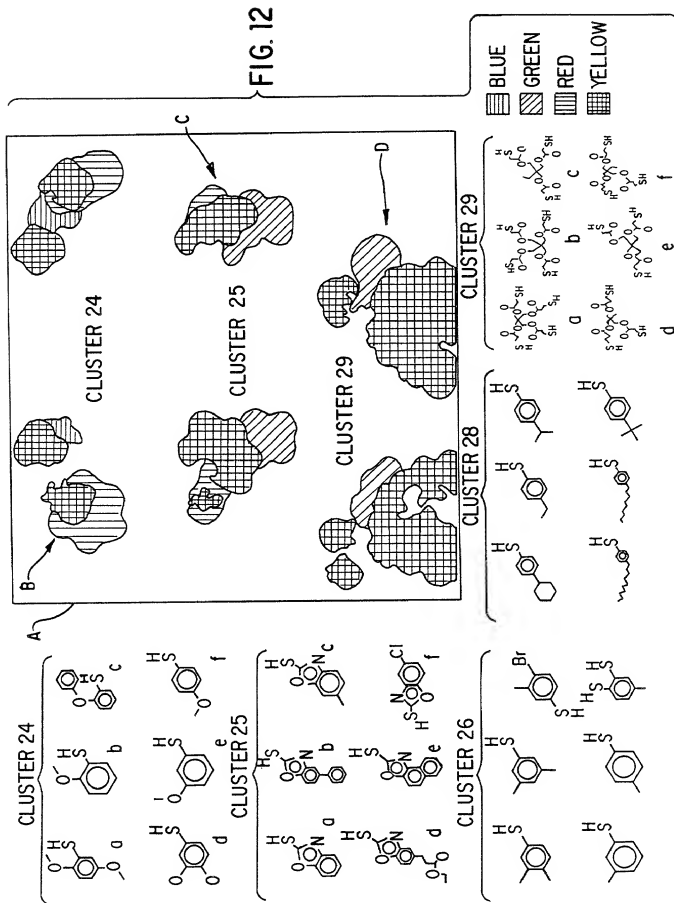


FIG.11(c)



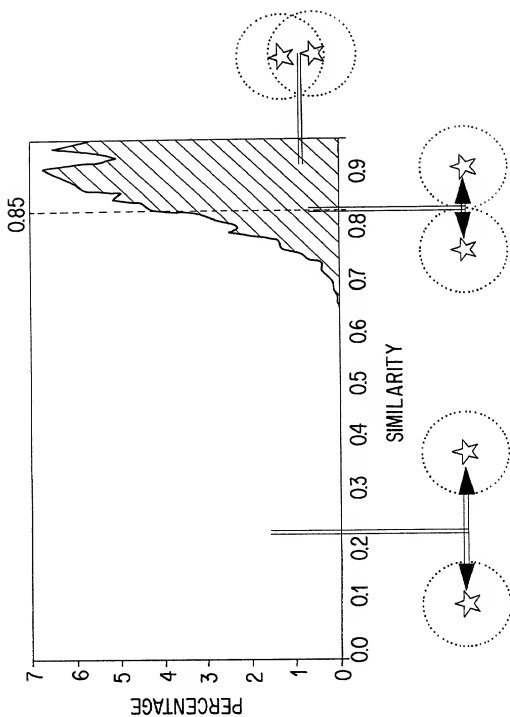


FIG.13

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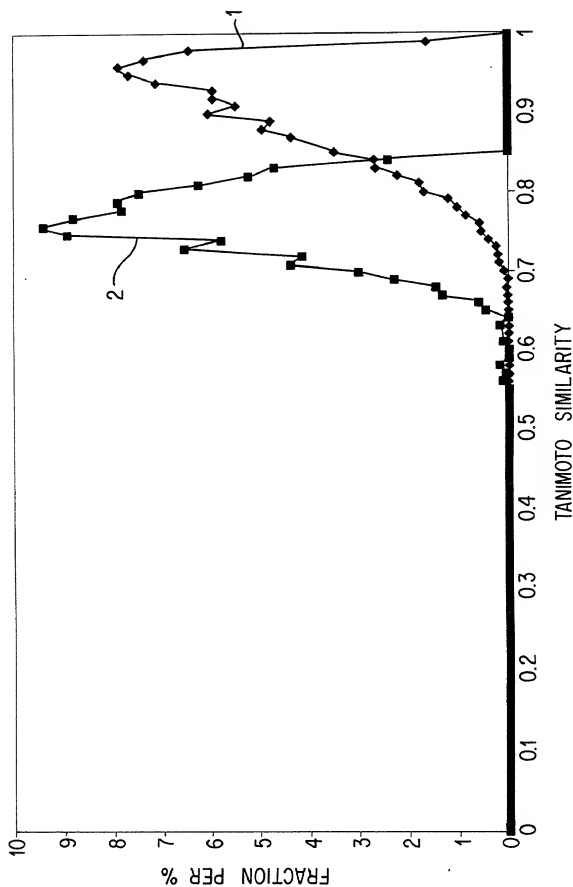


FIG. 14

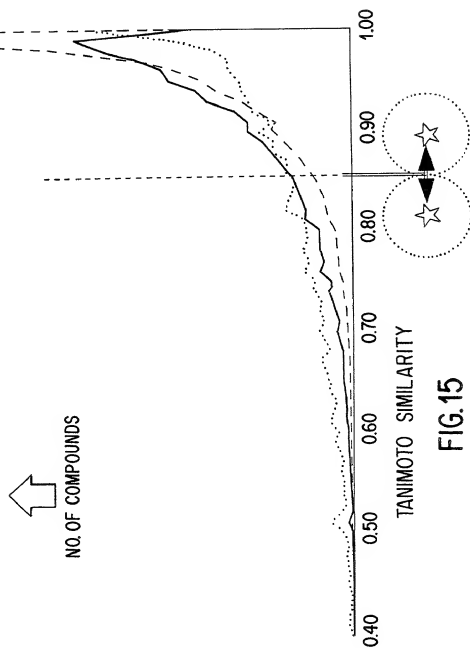


FIG. 15

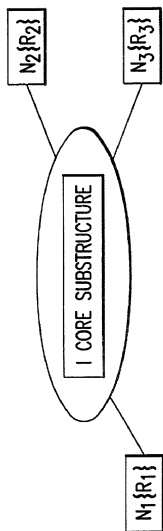


FIG.16

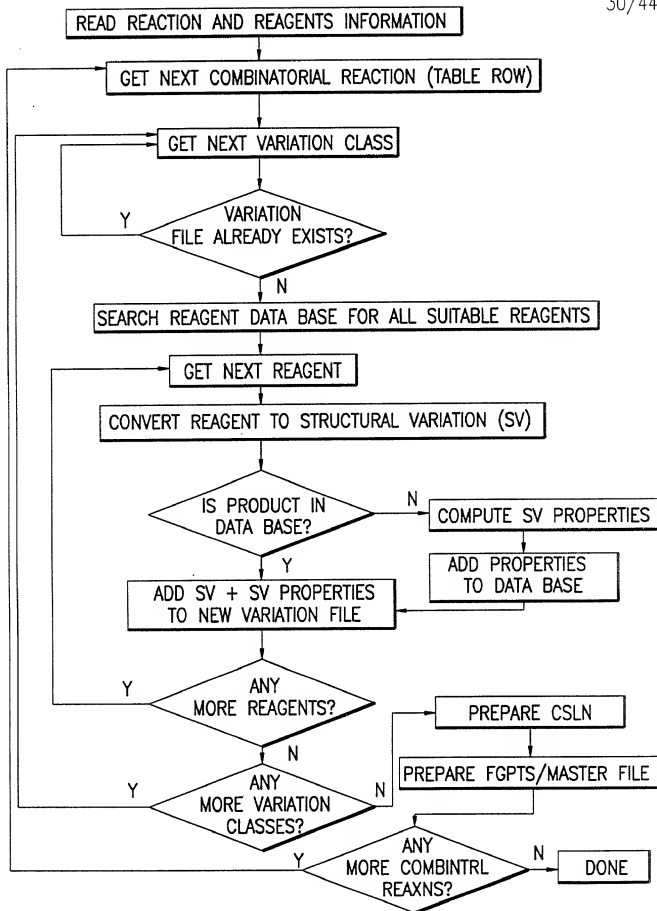


FIG.17

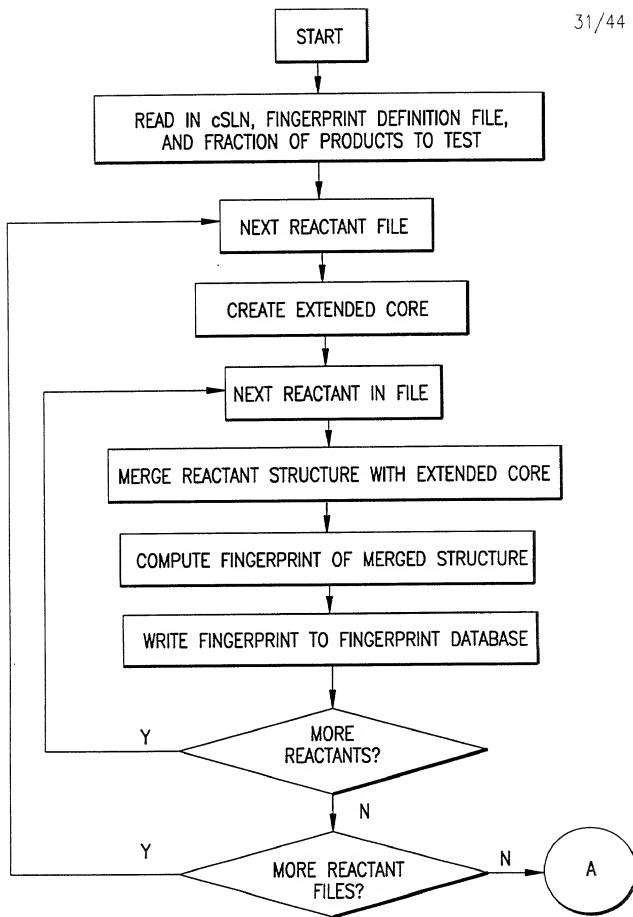


FIG.18

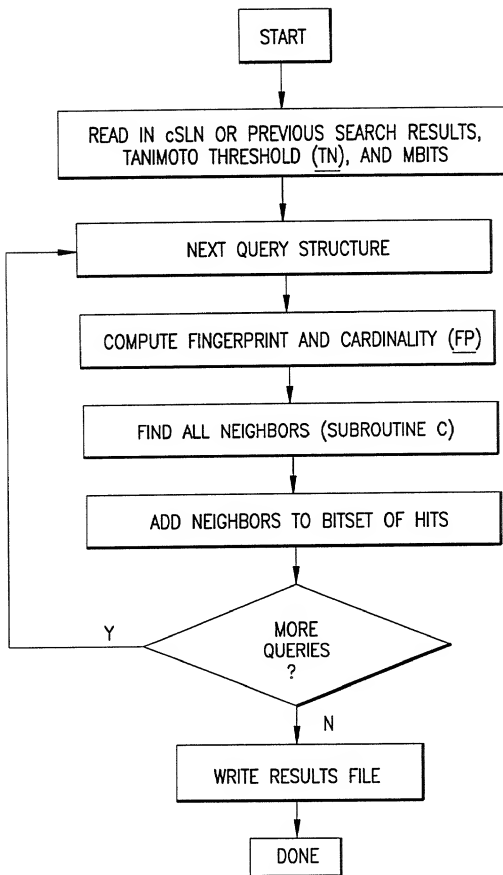


FIG.21

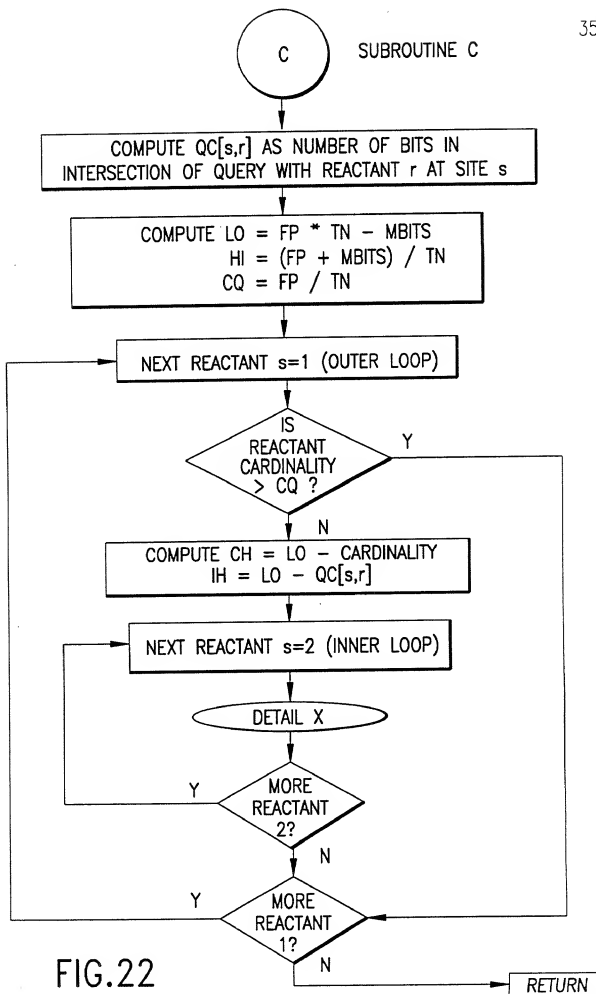


FIG.23

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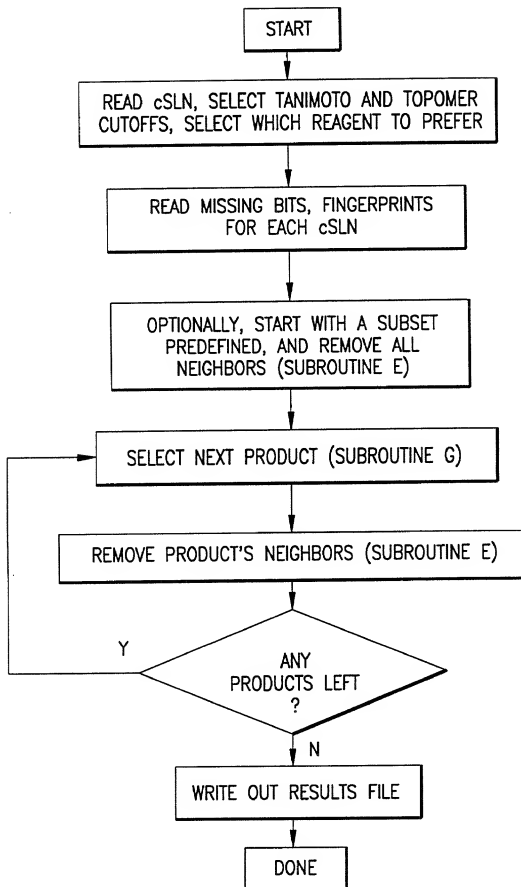


FIG.24

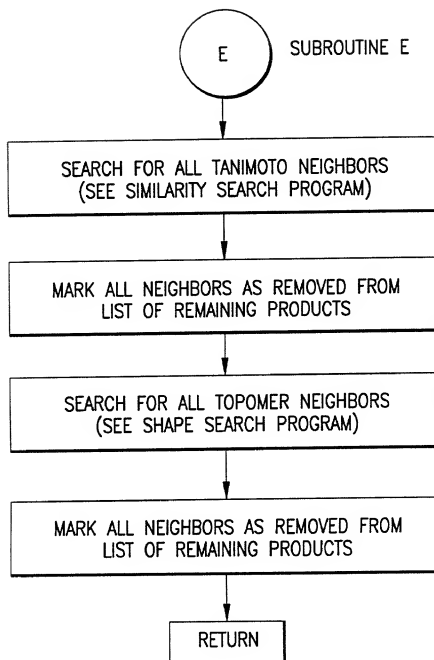
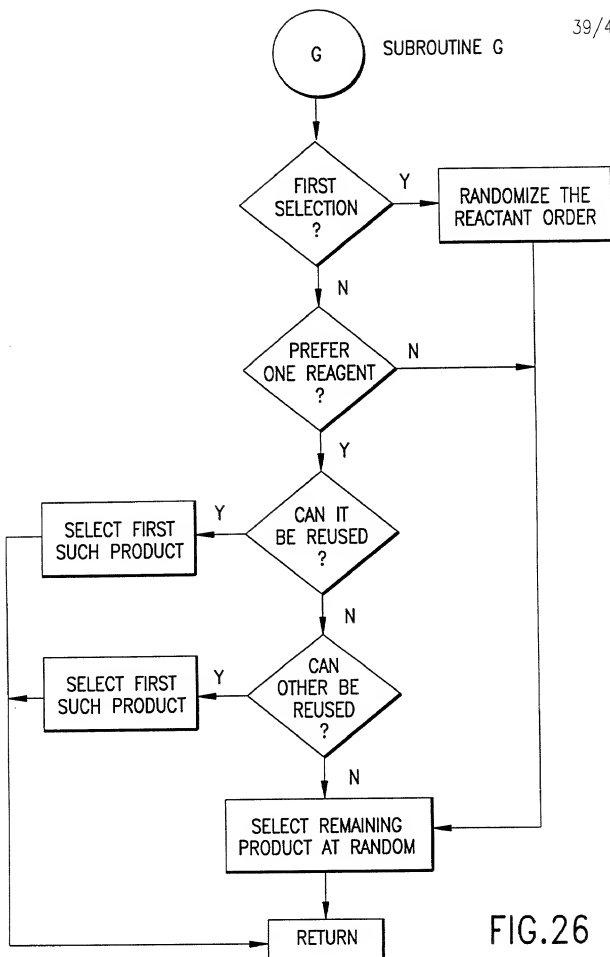


FIG.25

Abstract



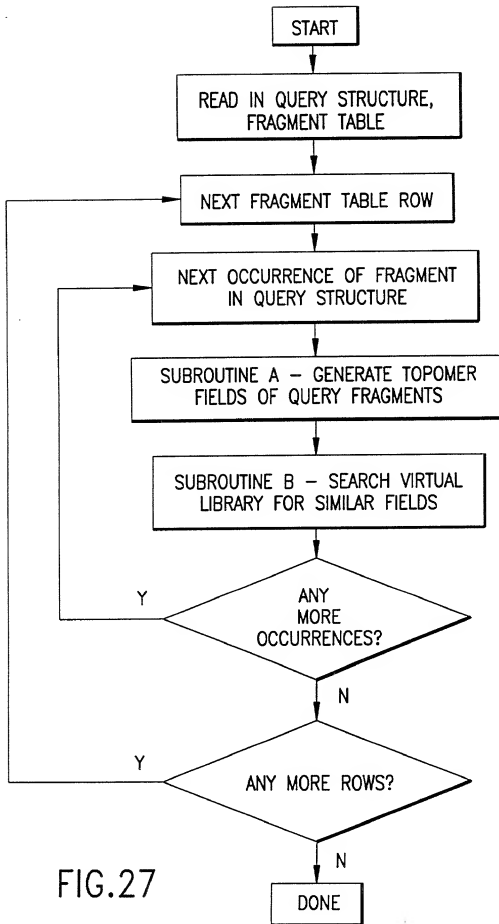


FIG.27

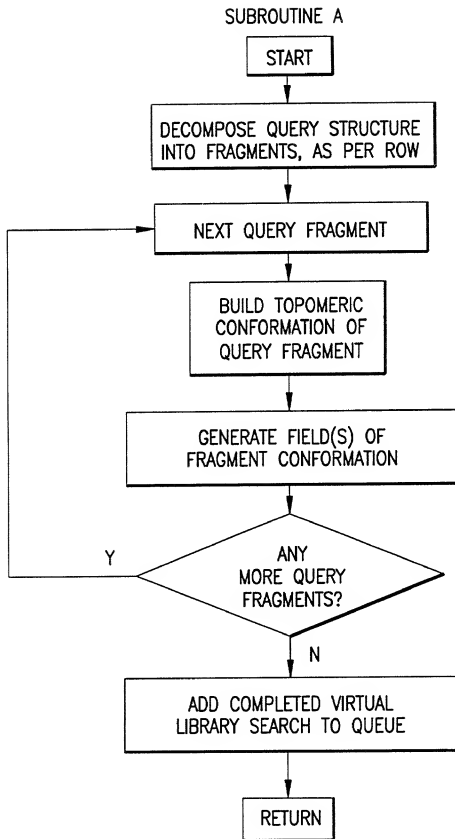


FIG.28

SUBROUTINE B

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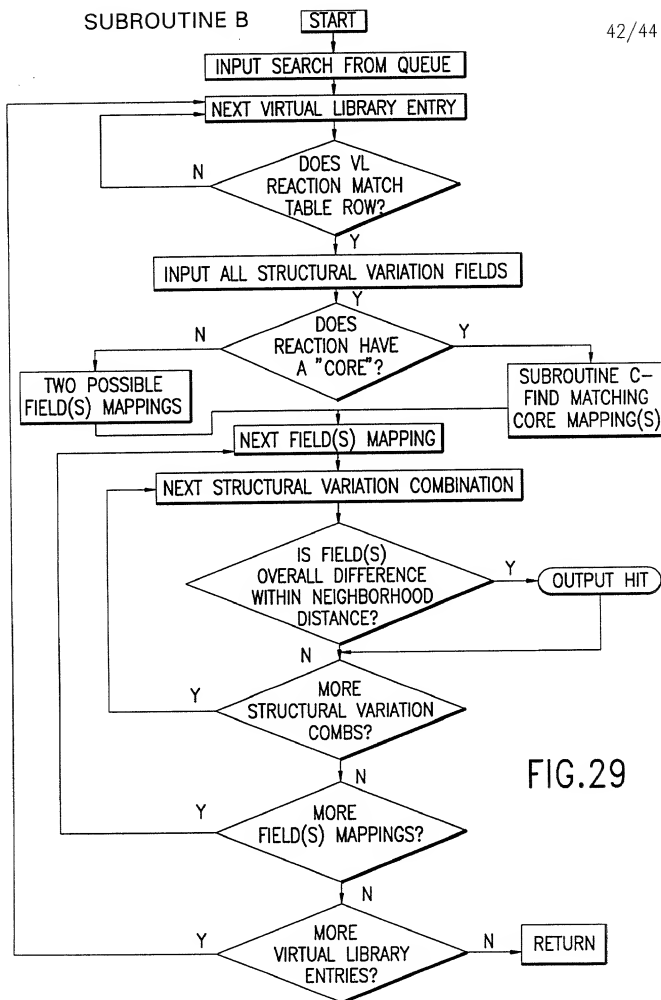


FIG.29

0000495.052501
100250.549890

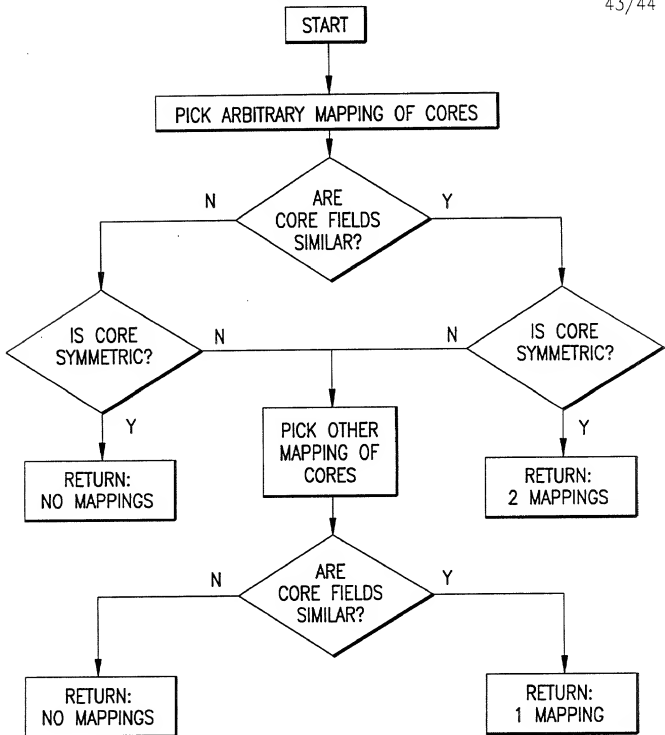


FIG.30

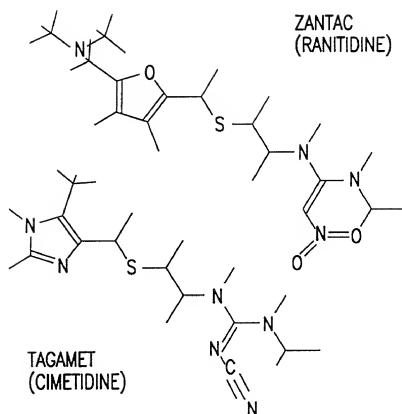


FIG.31